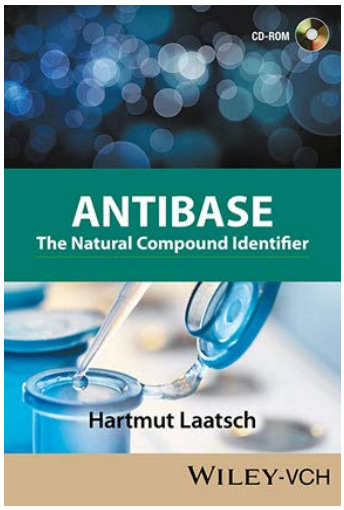
AntiBase: The Natural Compound Identifier

Hartmut Laatsch



Focused antimicrobial research through high-throughput screening library

Developed by Dr. Hartmut Laatsch, *AntiBase: The Natural Compound Identifier* is a compilation of natural products featuring properties of more than 40,000 compounds and over 41,000 chemical structures. This indispensable database provides researchers with a convenient way of checking if a compound with antimicrobial effects has already been studied and provides insights into biological activity correlated to structural information.

AntiBase includes compound property (molecular formula, mass, elemental composition, compound class), physico-chemical (melting point, optical rotation) and spectroscopic data (UV, 13C-NMR, IR, HRMS and mass spectra). Data has been collected from the primary and secondary literature, and then carefully checked and validated with most key references and source information provided as a data field.

Another unique feature of *AntiBase* is access to predicted 13C-NMR spectra for compounds in which no measured spectra are available. As an NMR shift search can easily be combined with a substructure search, this spectral data further enhances the power of *AntiBase* to easily differentiate between similar compounds. The predicted, high-quality NMR spectra were produced by Wiley's proprietary NMR spectrum prediction algorithm.

Library Specifications

- Natural Product Compounds: 40,004
- Chemical Structures: 41,047
- Spectra: 44,198
- Compound classification data: 10,227
- Source/Origin data: 41,307
- H-NMR spectra data: 629
- HRMS values for ion types (-H,+H,+Na): 41,048
- Optical Rotation (OR) values: 7,119
- Melting point data: 5,566

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Compatibility

- ISIS/Base
- PerkinElmer ChemFinder
- Agilent PCDL
- Bio-Rad ChemWindow*
- ACD/Labs ACD/Spectrus Processor*

*Subscription required

Compound Coverage

Compound coverage can be searched at www.compoundsearch.com.

Compound coverage includes:

- Algae
- Animals
- Bacteria
- Cyanobacteria
- Dinoflagellate
- Fungi
- Lichens
- Myxobacteria
- Plants
- Protozoan
- Slime mold
- Yeast

Ordering Information

Antibase: The Natural Compound Identifier
DVD-ROM ISBN: 978-3-527-34359-1

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